Benzamide, 2-chloro-n-(cyanomethyl)-n-cyclohexyl-4-nitro-

Inchi: InChI=1S/C15H16ClN3O3/c16-14-10-12(19(21)22)6-7-13(14)15(20)18(9-8-17)11-4-2-1-3

InchiKey: DUKMGBUPFGNRBQ-UHFFFAOYSA-N

Formula: C15H16ClN3O3

SMILES: N#CCN(C(=O)c1ccc([N+](=O)[O-])cc1Cl)C1CCCCC1

Mol. weight [g/mol]: 321.76

CAS: 22977-95-3

Physical Properties

Property code	Value	Unit	Source
gf	331.68	kJ/mol	Joback Method
hf	8.31	kJ/mol	Joback Method
hfus	41.39	kJ/mol	Joback Method
hvap	93.26	kJ/mol	Joback Method
log10ws	-5.34		Crippen Method
logp	3.547		Crippen Method
mcvol	230.180	ml/mol	McGowan Method
pc	2181.56	kPa	Joback Method
tb	956.45	K	Joback Method
tc	1216.69	K	Joback Method
tf	638.57	K	Joback Method
vc	0.881	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	700.78	J/mol×K	956.45	Joback Method
cpg	711.65	J/mol×K	999.82	Joback Method
cpg	721.31	J/mol×K	1043.20	Joback Method
cpg	729.86	J/mol×K	1086.57	Joback Method
cpg	737.40	J/mol×K	1129.94	Joback Method
cpg	744.03	J/mol×K	1173.31	Joback Method
cpg	749.84	J/mol×K	1216.69	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22977953&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume